

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY

NATIONAL EXPOSURE RESEARCH LABORATORY RESEARCH TRIANGLE PARK, NC 27711

OFFICE OF
RESEARCH AND DEVELOPMENT

June 10, 2019

Mr. Clark Freise, Assistant Commissioner New Hampshire Department of Environmental Services (NHDES) 29 Hazen Drive P.O. Box 95 Concord, New Hampshire 03301

Dear Mr. Freise:

I am pleased to provide the enclosed 6th report from our ongoing collaborative technical support to NHDES assisting with concerns over per- and polyfluorinated alkyl substances (PFAS) environmental contamination associated with manufacturing sites. This report is in response to your October 2017 request asking for laboratory assistance analyzing per- and polyfluoroalkyl substances (PFAS) in stack emissions and stock solutions of dispersions and surfactants. The enclosed Report #6 provides non-targeted analysis laboratory results that tentatively identify various PFAS found in the Modified Method 5 (MM5) process emissions samples collected from select runs of the QX, MS, and MA towers.

It is our understanding that this information was requested by NHDES to help in their ongoing investigation into the presence of PFAS in the environment near manufacturing facilities of interest. This request relates to our research capabilities and interests applying targeted and non-targeted analysis methods for discovery of the nature and extent of PFAS environmental occurrence that may be potentially associated with industrial releases. EPA continues to develop analytical methods for many PFAS compounds in various media including some of those included in this report. We are providing the results of our analysis as they become available.

In this report, we provide PFAS tentative identification and semi-quantitative analytical results. We do not interpret exposure or risk from these values. EPA does not currently have health-based standards, toxicity factors, or associated risk levels for PFAS, other than perfluorooctanoic acid (PFOA), perfluorooctane sulfonate (PFOS), and perfluorobutanesulfonic acid (PFBS). While the data provided in the attached reports indicate the presence (or lack) of PFAS in the MM5 samples, we do not have sufficient information to offer interpretations related to human or environmental exposure and risk.

Thank you for inviting us to be part of this effort that helps to further both EPA's and New Hampshire's understanding of an important issue in the state. This is just one of many Agency efforts that demonstrates EPA's commitment to cooperative federalism. If you have any questions or concerns, do not hesitate to contact me at (919) 541-2107 or via email at watkins.tim@epa.gov or Tim Buckley at (919) 541-2454 or via email at buckley.timothy@epa.gov. I look forward to our continued work together.

Sincerely,

Timothy H Watkins
Timothy H. Watkins

Director

Enclosure

CC: Meghan Cassidy, USEPA, Region 1
Deb Szaro, USEPA, Region 1
Jennifer McLain, USEPA, OW
Jessica Kramer, USEPA, OW
Mike Koerber, USEPA, OAR
Jeff Morris, USEPA, OPPT
Betsy Behl, USEPA, OW
Andy Gillespie, USEPA, ORD
Timothy Buckley, USEPA, ORD
Alice Gilliland, USEPA, ORD
Lara Phelps USEPA, ORD

PFAS Environmental Contamination Associated with Manufacturing Sites in New Hampshire

Laboratory Data Report #6: Non-Targeted PFAS Measurements in MM5 Sample Trains

Background. The New Hampshire Department of Environmental Services (NHDES), in coordination with EPA Region 1, requested the Office of Research and Development's (ORD's) technical support in analyzing per- and polyfluoroalkyl substances (PFAS) in MM5 sampling trains collected from air emission stacks at a manufacturing site within the State of New Hampshire. NHDES assumed responsibility for the collection of samples and their shipment to the ORD laboratory. ORD was responsible for sample extraction and analysis. ORD's analysis and report team that contributed to this effort are listed in Table 1.

Table 1. EPA Office of Research and Development analysis and report team.

Responsibility	Personnel
MM5 sampling expertise	Jeff Ryan
Laboratory chemistry	James McCord, Dennis Tabor
Quality Assurance Review	Sania Tong Argao
Management coordination and review	Kate Sullivan, Myriam Medina-Vera, Tim Buckley
Report Preparation	Kate Sullivan, Tim Buckley

This 6th report includes non-targeted analysis (NTA) results for four MM5 sampling trains that were used to collect PFAS emissions from three separate process towers identified as QX, MA, and MS during Run 1 of the tests at an industrial site in New Hampshire. The QX tower had a pilot emissions control device (ECD) and for this tower, MM5 emissions samples were simultaneously collected at the inlet and the outlet of the control device for the purpose of evaluating the control efficiency. Samples were collected in August 2018. Each MM5 sampling train consists of multiple components including a front half filter (FHF), an XAD trap (XAD), three impingers in series, and a back half filter (BHF). There is also a methanol rinse (MeOH) sample component resulting from rinse of the front half of the train components. Each MM5 train component is extracted and analyzed separately, and results in 7 individual MeOH extracts for analyses. Results for this report are limited to the FHF, XAD, and BHF components of the MM5 sampling train where we expect the bulk of the PFAS to be captured. The results from the impinger and MeOH rinsate samples will be reported at a later time. Accordingly, we provide results for 12 samples (4 MM5 trains x 3 sample components/MM5 train = 12 sample components) in this report. In addition to the MM5 sample results, we also report results for 4 process blanks. The samples were sent to ORD's laboratory in Research Triangle Park, NC where they were extracted by Dennis Tabor and analyzed for PFAS under the direction of Dr. James McCord.

The current data report is intended to provide a simple representation and summary of the analysis results. Therefore, the description of methods and quality assurance are brief and high-level. Additional reports and/or publications may be developed that will include a more detailed description of methods, quality assurance procedures, and statistical interpretation of the data. As study partners/collaborators, we anticipate that NHDES and Region 1 will assist in these reports and publications.

Methods in Brief. The PFAS reported here were extracted and analyzed according to methods documented within an approved Quality Assurance Project Plan (QAPP)¹ and described in McCord et al. 2019.² In brief, the MM5 methanolic extracts were vortexed as received and diluted 50:50 with 2mM ammonium formate in water for liquid chromatography-mass spectrometry (LC-MS) analysis. LC-MS analysis was carried out on a Thermo Vanquish ultra-performance liquid chromatograph (UPLC) system coupled to a Thermo Orbitrap Fusion mass spectrometer. PFAS were analyzed using non-targeted analysis (NTA) methods. Non-targeted analysis provides two important measurements. The first is a tentative identification of PFAS compounds detected in the sample. PFAS are tentatively identified based on a combination of mass spectral data along with patterns of fragmentation compared to on-line and in-house mass-spectral libraries. Analytes in each sample and process blank were identified to various levels of confidence depending on how much combined evidence from manual examination of MS/MS fragmentation spectra and/or comparison with mass spectral libraries.

The second measurement is an indication of how much of the PFAS was present in the sample. The mass spectrometer detector provides integrated peak areas for the chromatogram of the compound mass (+/- 5ppm) at the specified retention time. The peak area counts are proportional to the mass of PFAS in the sample. Since the sample and injection volume are held constant, the peak area counts are also proportional to concentration. However, without a standard, we are not able to derive a mass or concentration value and results are considered semi-quantitative. Accordingly, we provide sample results as peak area counts. It is important to emphasize that instrument response is highly variable among analytes and between samples.

The non-targeted analytical data set generated by LC/MS are considered as a "detect" when acceptable chromatographic peaks and spectra were evident. We used a variety of process blanks to account for any PFAS contamination that may have occurred during sampling and analysis including trip, laboratory, and instrument blanks. Process blanks are important for evaluating processing and/or solvent contamination that is not attributable to the samples. Our peak area detection limit is established based on PFAS measured in laboratory and trip blanks provided to us. We report non-detect (ND) for peak areas that are <5 times the mean value observed in the corresponding laboratory or trip blanks.

Summary of Results. Across all the MM5 samples, we detected and tentatively identified 190 different PFAS. Of those, we have high confidence in the tentative identification of 89 compounds, which we report by formula, chemical compound name and CAS number where available, and monoisotopic mass (Table 2). All of these compounds have tentative formulas, but most of the identified PFAS are novel as indicated by the lack of a CAS registry number (n=83; 93%), or lack of compound name (n=60, 67%). Some of these PFAS may be registered in EPA's CompTox dashboard where additional information can be found (U.S. EPA CompTox, 2019)³.

¹ National Exposure Research Laboratory, Quality Assurance Project Plan: Non-Targeted Analyses of Per- and Polyfluoroalkyl Substances (PFAS) for New Hampshire Department of Environmental Services (NHDES), October 2, 2017.

² McCord, J., Strynar, M. Identifying Per- and Polyfluorinated Chemical Species with a Combined Targeted and Non-Targeted-Screening High-Resolution Mass Spectrometry Workflow. *J. Vis. Exp.* (146), e59142, doi:10.3791/59142 (2019). https://www.jove.com/video/59142/identifying-per-polyfluorinated-chemical-species-with-combined

³ U.S. EPA CompTox Chemicals Dashboard https://comptox.epa.gov/dashboard

In Table 3 we provide semi-quantitative results for the 89 PFAS found in the MM5 methanol extracts and corresponding trip blanks and instrument blank for the analytes identified in Table 2. Sample peak area counts are superimposed on a heat map where gradations in color reflect seven classifications of peak area from low (non-detect) to high (>1,000,000). The heat map is useful in showing the samples where PFAS was detected and their relative peak areas.

For both Tables 2 and 3, PFAS are ordered by largest to smallest peak area counts based on the QX tower ECD inlet XAD sample (702). The PFAS measured included chain lengths from C2 to C36 with the majority between C5 and C16. Most of the PFAS emissions, both in terms of the number of compounds and peak area counts, came from the QX tower. A comparison of inlet to outlet PFAS measurements at the pilot ECD suggests an attributable modest reduction across most of the PFAS, varying by analyte. Fewer PFAS and much lower peak areas were observed for PFAS measured at the MA and MS towers.

In summary, we tentatively identified and semi-quantified 89 PFAS from MM5 samples collected at emission towers at a manufacturing site in NH. Many of the PFAS are likely novel evident from predominantly absent CAS numbers. The QX tower stood out in terms of the frequency of PFAS detection and where the highest peak areas tended to occur.

Table 2. Tentatively identified PFAS measured in MM5 samples.

Tentatively Identified Compound Name	Formula	Monoisotopic Mass (g/mol)
6:1 Fluorotelomer ether alcohol (formate adduct); CAS 376-93-2	C8 H5 F13 O4	411.9980
6:2 Fluorotelomer Unsaturated Carboxylic Acid (6:2 FTUCA)	C8 H2 F12 O2	357.9862
In-Source fragment, from 6:2 FTUCA	C7 H F11	293.9901
Perfluorohexanoic acid (PFHxA)	C6 H F11 O2	313.9799
In-Source fragment, from Perfluorohexanoic acid	C5 H F11	269.9903
Unknown	C15 H6 F22 O2	636.0020
6:2 Fluorotelomer ethoxycarboxylate (6:2 FTEOC); CAS 147011-35-6	C10 H7 F13 O3	422.0189
Perfluoroheptanoic acid (PFHpA)	C7 H F13 O2	363.9771
6:1 Fluorotelomer ether alcohol (formate adduct); CAS 1452584-51-8	C9 H7 F13 O3	410.0189
6:1 Fluorotelomer alcohol	C7 H3 F13 O	349.9975
Unknown	C12 H11 F13 O4	466.0454
Unknown	C20 H29 F13 O4	580.1864
Perfluoropentanoic acid (PFPeA)	C5 H F9 O2	263.9835
	C8 H5 F13 O3	396.0036
	C8 H3 F13 O2	377.9928
Unknown	C8 H4 F11 N O	339.0120
Perfluoropropanoic acid (PFPA)		163.9899
Unknown		627.9610
Unknown		514.0676
		213.9867
		510.0722
		513.0647
		661.9820
		402.0127
		468.0248
		586.1247
		345.9866
		554.0988
		261.9881
		398.0382
		345.9628
		261.9877
		723.9798
		400.0545
		588.1192
		438.0331 468.0804
		398.0382
		611.1920
		374.0219
		212.1778
		444.0801
		438.0694
		424.0540
i ritiuoroacetic acid		113.9933
Unknown	C22 H47 F N4 O5	466.3508
	6:1 Fluorotelomer ether alcohol (formate adduct); CAS 376-93-2 6:2 Fluorotelomer Unsaturated Carboxylic Acid (6:2 FTUCA) In-Source fragment, from 6:2 FTUCA Perfluorohexanoic acid (PFHxA) In-Source fragment, from Perfluorohexanoic acid Unknown 6:2 Fluorotelomer ethoxycarboxylate (6:2 FTEOC); CAS 147011-35-6 Perfluoroheptanoic acid (PFHpA) 6:1 Fluorotelomer ether alcohol (formate adduct); CAS 1452584-51-8 6:1 Fluorotelomer alcohol Unknown Unknown Perfluoropentanoic acid (PFPeA) 6:1 Fluorotelomer Alcohol (formate adduct) 2-Perfluorohexyl ethanoic acid; 6:2 FTA Unknown Perfluoropropanoic acid (PFPA)	6:1 Fluorotelomer ether alcohol (formate adduct); CAS 376-93-2 6:2 Fluorotelomer Unsaturated Carboxylic Acid (6:2 FTUCA) C7 H F11 Perfluorohexanoic acid (PFHXA) C6 H F11 02 In-Source fragment, from 6:2 FTUCA C7 H F11 Perfluorohexanoic acid (PFHXA) C6 H F11 02 In-Source fragment, from Perfluorohexanoic acid Unknown C15 H 6F22 02 C6:2 Fluorotelomer ethoxycarboxylate (6:2 FTEOC); CAS 147011-35-6 C10 H7 F13 03 Perfluoroheptanoic acid (PFHpA) C7 H F13 02 C6:1 Fluorotelomer ether alcohol (formate adduct); CAS 1452584-51-8 C9 H7 F13 03 C7 H F13 03 C7 H F13 03 C7 H F13 00 Unknown C12 H11 F13 04 Unknown C12 H11 F13 04 Unknown C20 H29 F13 04 Perfluoropentanoic acid (PFPA) C5 H F9 02 C6:1 Fluorotelomer Alcohol (formate adduct) C8 H5 F13 03 2-Perfluorohexyl ethanoic acid; 6:2 FTA C8 H3 F13 02 Unknown C8 H4 F11 N O Perfluoropropanoic acid (PFPA) C3 H F5 02 Unknown C12 H2 F22 04 Unknown C12 H2 F22 04 Unknown C12 H2 F22 04 Unknown C12 H2 F22 05 Unknown C12 H2 F22 05 Fluorotelomer ethoxycarboxylate C14 H15 F13 05 Unknown C15 H14 F11 N O6 Unknown C16 H4 F22 03 Unknown C16 H4 F22 03 Unknown C17 H23 F13 07 L-H Perfluoroheptanoic Acid C7 H2 F12 02 Unknown C10 H6 F12 03 Unknown C10 H6 F12 03 Unknown C11 H9 F13 05 Fluorinated ethoxycarboxylate C17 H23 F13 07 L-H Perfluoroheptanoic Acid C7 H2 F12 02 Unknown C16 H4 F24 03 Unknown C17 H2 F11 05 Fluorotelomer Methacrylate Unknown C18 H4 F24 03 Unknown C19 H6 F12 05 C5 Fluorotelomer Methacrylate Unknown C19 H7 F11 03 Unknown C19 H7 F11 03 Unknown C19 H7 F11 05 Unknown C

Compound #	Tentatively Identified Compound Name	Formula	Monoisotopio Mass (g/mol)
48	Unknown	C24 H44 O20	652.2444
49	Unknown	C13 H7 F23 O3	648.0025
50	Unknown	C11 H10 F14 N4 O3	512.0513
51	Unknown	C15 H15 F11 O3	452.0853
52	2H,2H,3H,3H-Perfluorooctanoic acid	C8 H5 F11 O2	342.0117
53	Adduct or parent of 643.99542	C15 H4 F23 N5 O	707.0031
55 	8:2 Fluorotelomer sulfonic acid	C10 H5 F17 O3 S	527.9683
55	Unknown	C9 H5 F11 O3	370.0065
56	Unknown	C10 H7 F17 N4 O13	713.9754
57	Unknown	C16 H20 F14 N4 O4	598.1253
58	1-H Perfluorohexanoic acid	C6 H2 F10 O2	295.9895
59	Unknown	C12 H6 F24 N4 O2	694.0091
60	Unknown	C10 H7 F13 O4	438.0142
61	Unknown	C6 H5 F9 O4	312.0048
62	Unknown	C11 H14 F12 O4	438.0694
63	Unknown	C22 H19 F27 N4 O5	932.0918
64	Unknown	C32 H47 F13 N4 O7	846.3238
65	Unknown	C12 H10 F14 N4 O3	524.0518
66	Unknown	C20 H29 F7 N2 O7 S	574.1593
67	Unknown	C5 H3 F11 N4 O	344.0125
68	Unknown	C7 H4 F10 O4	341.9951
69	Unknown	C13 H11 F11 O3	424.0540
70	PFECA; CAS 919005-00-8	C5 H2 F8 O3	261.9882
71	Unknown	C15 H15 F11 O3	452.0853
72	Unknown	C10 H9 F11 O3	386.0380
73	Unknown	C12 H8 F24 N4 O	680.0286
74	Unknown	C36 H61 F13 O13	948.3913
75	Unknown	C6 H5 F11 O3	334.0064
76	Perfluorononanoic acid (PFNA)	C9 H F17 O2	463.9713
77	Unknown	C14 H14 F12 N4	466.1012
78	Unknown	C13 H18 F12 O5	482.0960
79	Unknown	C10 H F14 N O2	432.9790
80	Unknown	C11 H9 F11 O3	398.0382
81	Unknown	C8 H5 F11 O3	358.0062
82	Unknown	C15 H6 F22 O3	651.9987
83	Unknown	C10 H9 F11 O3	386.0380
84	Unknown	C15 H22 F12 O5	510.1283
85	Unknown	C8 H7 F11 O4	376.0170
86	Unknown	C15 H9 F23 N4 O3	730.0294
87	Perfluorooctanoic Acid (PFOA)	C8 H F15 O2	413.9744
88	Unknown	C8 H5 F12 N O4	407.0022
89	Unknown	C13 H4 F23 N O4	674.9776

Table 3. Detection and measurement of PFAS in MM5 samples. Results are reported as peak area units. Table cells are color-coded to indicate detection and peak area class.

		QX Tower (Inlet)		QX	Tower (Outl	et)		MA Towe	r		MS Towe	r	Blanks				
Formula	Compound #	QX Tower Inlet FH Filter (700)	QX Tower Inlet XAD (702)	QX Tower Inlet BH Filter (706)	QX Tower Outlet FH Filter (800)	QX Tower Outlet XAD (802)	QX Tower Outlet BH Filter (806)	MA Tower FH Filter (500)	MA Tower XAD (502)	MA Tower BH Filter (506)	MS Tower FH Filter (600)	MS Tower XAD (602)	MS Tower BH Filter (606)	Trip Blank FH Filter (200)	Trip Blank XAD (202)	Trip Blank BH Filter (205)	Laboratory (206)
C8 H5 F13 O4	1	70,500	66,400,000	88,100	ND	18,500,000	13,700	ND	ND	ND	ND	10,000	ND	ND	ND	ND	ND
C8 H2 F12 O2	2	399,000	51,800,000	110,000	354,000	9,270,000	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C7 H F11	3	210,000	26,000,000	54,000	173,000	4,000,000	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C6 H F11 O2	4	469,000	23,400,000	246,000	713,000	34,000,000	71,100	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C5 H F11	5	282,000	17,700,000	140,000	388,000	20,100,000	29,700	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C15 H6 F22 O2	6	ND	13,500,000	26,300	ND	5,840,000	6,030	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C10 H7 F13 O3	7	104,000	9,840,000	81,700	116,000	1,050,000	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C7 H F13 O2	8	47,800	7,080,000	63,000	121,000	656,000	3,370	3,540	ND	ND	ND	ND	ND	ND	ND	ND	ND
C9 H7 F13 O3	9	20,500	5,180,000	196	1,500	6,750,000	ND	ND	1,080	ND	ND	192	ND	ND	ND	ND	ND
C7 H3 F13 O	10	6,620	4,430,000	11,100	ND	1,260,000	1,210	ND	814	ND	ND	477	ND	ND	ND	ND	ND
C12 H11 F13 O4	11	95,400	3,800,000	154,000	59,600	11,500	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C20 H29 F13 O4	12	ND	3,330,000	223	ND	1,320,000	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C5 H F9 O2	13	231,000	3,040,000	104,000	518,000	ND	ND	ND	ND	ND	ND	ND	ND	ND	39,400	ND	ND
C8 H5 F13 O3	14	1,020	2,480,000	ND	ND	443,000	ND	ND	2,350	ND	ND	ND	ND	ND	ND	ND	ND
C8 H3 F13 O2	15	21,100	2,370,000	5,060	3,090	213,000	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C8 H4 F11 N O	16	9,300	2,140,000	1,630	ND	116,000	713	ND	1,230	ND	ND	731	ND	ND	ND	ND	ND
C3 H F5 O2	17	58,600	2,070,000	6,970	134,000	120,000	ND	ND	333,000	ND	ND	130,000	ND	ND	ND	ND	ND
C12 H2 F22 O4	18	14,800	2,030,000	4,510	43,900	1,960,000	231	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C11 H12 F14 N4 O3	19	28,900	1,770,000	8,390	1,890	73,600	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C4 H F7 O2	20	92,400	1,580,000	34,400	285,000	289,000	1,450	ND	2,850	ND	ND	ND	ND	ND	ND	ND	ND
C14 H15 F13 O5	21	81,900	1,470,000	76,300	12,600	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C15 H14 F11 N O6	22	28,700	1,440,000	1,560	ND	376,000	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C16 H4 F22 O3	23	ND	1,200,000	126	ND	1,890,000	211	ND	134	ND	ND	ND	ND	ND	ND	ND	ND
C10 H6 F12 O3	24	14,100	1,060,000	15,100	33,300	133,000	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C11 H9 F13 O5	25	9,130	915,000	19,800	41,100	116,000	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

		QX Tower (Inlet)			QX	QX Tower (Outlet)			MA Tower			MS Towe	r	Blanks			
Formula	Compound #	QX Tower Inlet FH Filter (700)	QX Tower Inlet XAD (702)	QX Tower Inlet BH Filter (706)	QX Tower Outlet FH Filter (800)	QX Tower Outlet XAD (802)	QX Tower Outlet BH Filter (806)	MA Tower FH Filter (500)	MA Tower XAD (502)	MA Tower BH Filter (506)	MS Tower FH Filter (600)	MS Tower XAD (602)	MS Tower BH Filter (606)	Trip Blank FH Filter (200)	Trip Blank XAD (202)	Trip Blank BH Filter (205)	Laboratory (206)
C17 H23 F13 O7	26	60,100	896,000	48,100	18,200	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C7 H2 F12 O2	27	5,030	820,000	2,080	72,400	32,100	ND	1,210	1,990	ND	ND	894	ND	ND	ND	ND	ND
C16 H19 F13 O6	28	72,800	619,000	39,000	5,420	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C5 H2 F8 O3	29	127,000	585,000	8,650	26,400	340,000	ND	ND	ND	ND	ND	18,600	ND	ND	ND	ND	ND
C11 H9 F11 O3	30	ND	439,000	ND	ND	50,200	ND	ND	1,370	ND	ND	819	ND	ND	ND	ND	ND
C7 H2 CI F11 O	31	124	428,000	ND	ND	194,000	ND	ND	267	ND	ND	211	ND	ND	ND	ND	ND
C5 H2 F8 O3	32	127,000	413,000	244,000	916,000	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C18 H4 F24 O3	33	390	381,000	2,620	ND	9,230	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C11 H11 F11 O3	34	ND	367,000	172	ND	143,000	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C18 H18 F14 N4 O2	35	ND	367,000	ND	ND	133,000	ND	ND	ND	ND	ND	1,230	ND	ND	231	ND	ND
C10 H10 F12 O5	36	ND	362,000	ND	ND	47,100	ND	ND	524	ND	ND	256	ND	ND	ND	ND	ND
C12 H16 F12 O5	37	ND	351,000	ND	ND	467,000	ND	ND	145	ND	ND	ND	ND	ND	ND	ND	ND
C11 H9 F11 O3	38	ND	300,000	ND	ND	142,000	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C18 H27 F14 N5 O2	39	ND	294,000	ND	ND	195,000	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C8 H8 F10 O5	40	4,310	291,000	755	66	60,600	ND	ND	85	ND	ND	523	ND	ND	ND	ND	ND
C13 H24 O2	41	10,700	291,000	ND	ND	ND	ND	ND	209,000	ND	ND	20,100	ND	ND	ND	ND	ND
C13 H15 F11 O4	42	ND	284,000	ND	ND	233,000	55	ND	168	ND	ND	ND	ND	ND	ND	ND	ND
C14 H13 F11 O3	43	ND	281,000	ND	ND	216,000	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C13 H11 F11 O3	44	ND	254,000	146	ND	16,900	ND	ND	924	ND	ND	ND	ND	ND	ND	ND	ND
C2 H F3 O2	45	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	198,000	ND	ND
C22 H47 F N4 O5	46	127,000	229,000	2,170	1,360	ND	ND	ND	ND	ND	ND	ND	ND	ND	529	ND	ND
C19 H27 F13 O4	47	ND	225,000	ND	ND	62,600	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C24 H44 O20	48	ND	214,000	ND	ND	175,000	362	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
C13 H7 F23 O3	49	ND	209,000	177	ND	106,000	ND	ND	230	ND	ND	ND	ND	ND	ND	ND	ND
C11 H10 F14 N4 O3	50	800	206,000	12,000	4,750	ND	ND	ND	ND	ND	ND	ND	ND	ND	441	ND	ND
C15 H15 F11 O3	51	ND	197,000	ND	ND	168,000	ND	ND	125	ND	ND	ND	ND	ND	ND	ND	ND
C8 H5 F11 O2	52	210	188,000	ND	ND	358,000	ND	ND	ND	ND	ND	ND	ND	ND	231	ND	ND

		QX Tower (Inlet)			QX Tower (Outlet)			MA Tower				MS Towe	r	Blanks				
Formula	Compound #	QX Tower Inlet FH Filter (700)	QX Tower Inlet XAD (702)	QX Tower Inlet BH Filter (706)	QX Tower Outlet FH Filter (800)	QX Tower Outlet XAD (802)	QX Tower Outlet BH Filter (806)	MA Tower FH Filter (500)	MA Tower XAD (502)	MA Tower BH Filter (506)	MS Tower FH Filter (600)	MS Tower XAD (602)	MS Tower BH Filter (606)	Trip Blank FH Filter (200)	Trip Blank XAD (202)	Trip Blank BH Filter (205)	Laboratory (206)	
C15 H4 F23 N5 O	53	ND	185,000	ND	ND	7,400	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
C10 H5 F17 O3 S	54	6,440	176,000	1,110	39,200	573	ND	ND	88	ND	ND	ND	ND	ND	ND	ND	ND	
C9 H5 F11 O3	55	6,630	170,000	7,550	14,600	406,000	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
C10 H7 F17 N4 O13	56	ND	161,000	ND	ND	23,300	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
C16 H20 F14 N4 O4	57	107,000	158,000	12,900	2,460	ND	ND	ND	1,100	ND	ND	ND	ND	ND	ND	ND	ND	
C6 H2 F10 O2	58	196	157,000	425	ND	165,000	ND	ND	ND	ND	ND	1,210	ND	ND	237	ND	ND	
C12 H6 F24 N4 O2	59	ND	155,000	171	ND	73,600	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
C10 H7 F13 O4	60	2,590	155,000	1,420	498	4,320	ND	ND	134	ND	ND	ND	ND	ND	ND	ND	ND	
C6 H5 F9 O4	61	ND	152,000	ND	ND	34,800	ND	ND	81	ND	ND	ND	ND	ND	ND	ND	ND	
C11 H14 F12 O4	62	147	150,000	ND	ND	79,100	ND	ND	184	ND	ND	ND	ND	ND	ND	ND	ND	
C22 H19 F27 N4 O5	63	ND	148,000	424	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	154	ND	ND	
C32 H47 F13 N4 O7	64	136	143,000	ND	ND	55,400	ND	ND	ND	ND	ND	ND	ND	ND	326	ND	ND	
C12 H10 F14 N4 O3	65	10,000	140,000	9,050	1,160	ND	ND	ND	ND	ND	ND	ND	ND	ND	690	ND	ND	
C20 H29 F7 N2 O7 S	66	523	139,000	ND	ND	4,770	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
C5 H3 F11 N4 O	67	515	133,000	ND	ND	123,000	ND	ND	188	ND	ND	612	ND	ND	ND	ND	ND	
C7 H4 F10 O4	68	83	127,000	ND	ND	118,000	ND	ND	ND	ND	ND	ND	ND	ND	237	ND	ND	
C13 H11 F11 O3	69	ND	125,000	129	ND	73,700	ND	ND	587	ND	ND	ND	ND	ND	ND	ND	ND	
C5 H2 F8 O3	70	ND	123,000	3,600	ND	340,000	ND	ND	ND	ND	ND	17,100	ND	ND	ND	ND	ND	
C15 H15 F11 O3	71	ND	122,000	ND	ND	97,500	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
C10 H9 F11 O3	72	326	120,000	85	ND	204,000	330	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
C12 H8 F24 N4 O	73	ND	119,000	131	ND	8,210	ND	ND	532	ND	ND	ND	ND	ND	ND	ND	ND	
C36 H61 F13 O13	74	ND	114,000	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	466	ND	ND	
C6 H5 F11 O3	75	ND	113,000	ND	ND	14,900	ND	ND	492	ND	ND	461	ND	ND	ND	ND	ND	
C9 H F17 O2	76	721	109,000	8,050	ND	5,110	ND	ND	ND	ND	ND	2,260	ND	ND	442	ND	ND	
C14 H14 F12 N4	77	ND	107,000	128	ND	397,000	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
C13 H18 F12 O5	78	ND	105,000	ND	ND	96,300	ND	ND	76	ND	ND	ND	ND	ND	ND	ND	ND	
C10 H F14 N O2	79	495	93,000	423	ND	158,000	1,030	ND	ND	ND	ND	ND	ND	ND	203	ND	ND	

		QX Tower (Inlet)			QX Tower (Outlet)			MA Tower			MS Tower			Blanks				
Formula	Compound #	QX Tower Inlet FH Filter (700)	QX Tower Inlet XAD (702)	QX Tower Inlet BH Filter (706)	QX Tower Outlet FH Filter (800)	QX Tower Outlet XAD (802)	QX Tower Outlet BH Filter (806)	MA Tower FH Filter (500)	MA Tower XAD (502)	MA Tower BH Filter (506)	MS Tower FH Filter (600)	MS Tower XAD (602)	MS Tower BH Filter (606)	Trip Blank FH Filter (200)	Trip Blank XAD (202)	Trip Blank BH Filter (205)	Laboratory (206)	
C11 H9 F11 O3	80	ND	86,900	330	ND	194,000	ND	ND	184	ND	ND	138	ND	ND	ND	ND	ND	
C8 H5 F11 O3	81	1,420	86,500	ND	433	417,000	ND	ND	ND	ND	ND	ND	ND	ND	342	ND	ND	
C15 H6 F22 O3	82	ND	57,000	ND	ND	149,000	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
C10 H9 F11 O3	83	74	51,600	74	ND	278,000	219	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
C15 H22 F12 O5	84	ND	44,400	ND	ND	119,000	ND	ND	125,000	ND	ND	ND	ND	ND	ND	ND	ND	
C8 H7 F11 O4	85	1,020	35,600	163	309	412,000	ND	ND	ND	ND	ND	ND	ND	ND	214	ND	ND	
C15 H9 F23 N4 O3	86	ND	21,600	ND	ND	203,000	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	
C8 H F15 O2	87	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	69,500	ND	164,000	1,470	ND	
C8 H5 F12 N O4	88	ND	ND	ND	ND	274,000	ND	ND	ND	ND	ND	ND	ND	ND	878	ND	ND	
C13 H4 F23 N O4	89	ND	1,170	ND	ND	114,000	ND	ND	143	ND	ND	ND	ND	ND	ND	ND	ND	

LEGEND

CLITE	
Color	Peak Area as Relative Indicator of Abundance
ND	<5x Method Blanks or Trip Blanks
	>5x blank to 30,000
	30,000 - 50,000
	50,000 - 100,000
	100,000-400,000
	400,000 -1,000,000
	>1,000,000